OR-5. NEW APPROACH TO UNSYMMETRICAL 1,3- AND 1,4-DIAZATRIPHENYLENE DERIVATIVES THROUGH INTRAMOLECULAR OXIDATIVE CYCLODEHYDROGENATION

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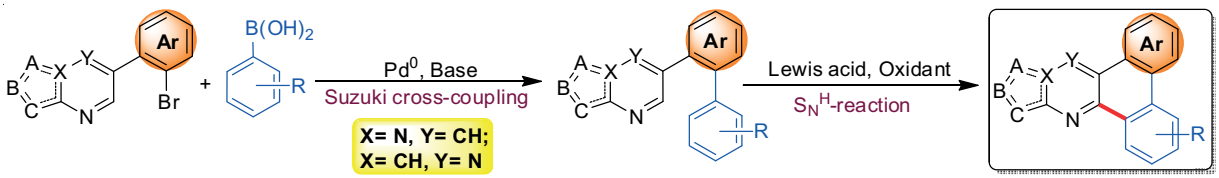
Polycyclic heteroaromatic compounds have received much attention as a fundamental framework in organic functional materials because their electrochemical and photochemical properties are useful in organic electronics and luminescent materials. Among them, 1,3- and 1,4-diazatriphenylene derivatives frequently appeared in molecular unit in the preparation of extended π-conjugated systems with characteristic optical and electrochemical properties [1].

Herein, we describe the synthesis of an unsymmetrical substituted dibenzo[*f*, *h*]quinazolines (**X=N**, **Y=CH**, **A=B=C** – not present) and dibenzo[*f*, *h*]furazano[3,4-*b*]quinoxalines (**X=A=C=N**, **Y=CH**, **B=O)** by the sequence of Suzuki cross-coupling reaction and intramolecular oxidative cyclodehydrogenation (S_N^H-reaction) [2]. The optimization of reaction conditions for each stage were produced.



The electrochemical and photophysical properties for several polycycles have been measured. In particular, dibenzo[*f*, *h*]furazano[3,4-*b*]quinoxalines possess hole mobility of the order of 10^{-4} $cm^2V^{-1}s^{-1}$ that make them perspective for fabrication of hole transport layer in perovskite solar cells, because their hole mobility values are close to the reference molecule spiro-OMeTAD and HOMO levels match well with that of $MAPbI_3$.

References

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